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Published in:
Physical Review B. Condensed Matter and Materials Physics

DOI:
10.1103/PhysRevB.57.R8127

Publication date:
1998

Document version
Early version, also known as pre-print

PHYSICAL REVIEW B VOLUME 57, NUMBER 14 1 APRIL 1998-II

Intrinsic temperature dependences of transport coefficients within the hot-spot model for normal-state $YBa_2Cu_3O_7$

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(Received 22 December 1977)

The temperature dependences of the galvanomagnetic and thermoelectric transport coefficients within a generic *hot-spot* model are reconsidered. Despite the recent success in explaining ac Hall effect data in $YBa_2Cu_3O_7$, a general feature of this model is a departure from the approximately universal temperature dependences observed for normal state transport in the optimally doped cuprates. In this paper, we discuss such systematic deviations and illustrate some of their effects through a concrete numerical example using the calculated band structure for $YBa_2Cu_3O_7$. [S0163-1829(98)51512-3]

The construction of a consistent phenomenology for normal state transport in the cuprates has turned out to be highly problematic. At an early stage it was suggested by Anderson[1] that experimental magnetotransport data should be fitted using two distinct relaxation rates, and plentiful experimental verifications have by now made this conjecture an attractive ansatz for interpreting normal state transport data. Thus, in pure optimally doped $YBa_2Cu_3O_7$, resistivity and inverse Hall angle have been successfully related to the two relaxation rates

$$1/\tau_{tr}=\eta T, \quad 1/\tau_H=T^2/W_H \tag{1}$$

proving to be valid over a substantial range of temperatures.[2] The prefactor η may be inferred from the width of the ac conductivity peak to be ~ 2,[3] while the energy scale W_H is less agreed upon. The original Anderson proposal related W_H to the spinon bandwidth, of the order of the superexchange energy $J\sim 1400$ K, which is in reasonable accordance with an experimental fit by Chien *et al.*,[4] who found W_H to be 830 K. This value however presupposes a connection between W_H and the cyclotron frequency, and as pointed out in Ref. 5, the same data yield $W_H\sim 65$ K or less, if in the cyclotron frequency one uses simply the mass deduced from the optical conductivity. The latter interpretation complies well with the ac magnetotransport data of Drew *et al.*[6,7] suggesting that $W_H\sim 120$ K.

Various phenomenologies have been suggested as underlying this experimentally appealing concept of two relaxation rates, but, as pointed out in a recent work by Coleman, Schofield, and Tsvelik,[8] most of these suggestions are problematic in one way or the other. They pointed to the fact that electrical current and Hall current have opposite parity under charge conjugation, which seems to indicate that some as yet unknown scattering mechanism sensitive to charge conjugation is at play. Their Majorana fermion Boltzmann equation yields a set of transport coefficients, in which the scattering rates combine in *series* or *parallel*, making either the smallest or the largest of the two dominant and therefore it relies on a marked difference in magnitude of the two rates. A particularly interesting consequence of this phenomenology is the fact that the thermopower turns out to be simply related to the Hall constant as

$$\frac{S}{T}=a+bR_H, \tag{2}$$

implying that a longitudinal current, such as the response to a temperature gradient, may also be related to the Hall scattering rate. This appears to be consistent with thermoelectric experiments in thin films of $Tl_2Ba_2CaCu_2O_{8+\delta}$,[9] supporting the idea that the two relaxation rates do not pertain to transverse and longitudinal currents respectively, but rather to currents of even or odd charge conjugation parity.

In the course of fitting ac Hall effect data the standard Bloch-Boltzmann theory based on band-structure calculations and angle-resolved photoemission experiments, supplied by the assumption of an anisotropic relaxation rate, has been reconsidered recently by Zheleznyak, Yakovenko, Drew, and Mazin.[10] They have elaborated on what they name the *additive* two-τ approach taken earlier by Carrington *et al.*[11] and Kendziora *et al.*,[12] where the relaxation rate was assumed to have different temperature dependences on different parts of the Fermi surface. The notion of an anisotropic relaxation rate has been applied succesfully in explaining the observed deviations from nearly free electron values of the Hall constant in Al and Pd,[13] and seems as a natural minimal model to explain abnormal transport data. However, as the present Communication is meant to demonstrate, this approach leads to temperature dependences which are largely inconsistent with normal state transport experiments in optimally doped cuprates.

The authors of Ref. 10 have mainly focused on frequency dependences, and for this purpose indeed the additive two-τ model works rather well. Their analysis was based on the band-structure calculations for $YBa_2Cu_3O_7$ by Andersen *et al.*,[14] supplied with the assumption that the relaxation rate has linear temperature dependence on the flat parts and quadratic temperature dependence on the corners of the Fermi surface. Only the in-plane bonding band was considered

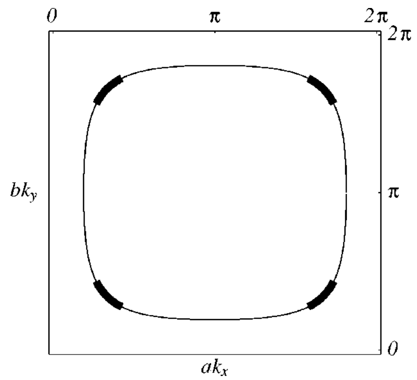

FIG. 1. Even plane band Fermi surface for $YBa_2Cu_3O_7$, from Ref. 14. In the text, flat parts (thin lines) and corners are referred to by subscripts f and c, respectively.

since it was found to have the largest contribution to the conductivities. With the parameters given in Ref. 14 for this even plane band, the resulting Fermi surface has been replotted in Fig. 1 and the notion of flat parts and corners are seen to be easily resolved. Continuing along the lines of Ref. 10, we now want to focus on temperature rather than frequency dependences.

Within the *momentum independent* relaxation time approximation, a standard solution of the Boltzmann equation for a square symmetric 2D system (neglecting the slight anisotropy of $YBa_2Cu_3O_7$) yields the following low temperature and low field longitudinal, Hall, thermoelectric and transverse magnetoconductivity:

$$\sigma=\left(\frac{e}{2\pi}\right)^2\oint dk_{\parallel}v_i\delta_{ij}v_j\tau/v, \tag{3}$$

$$\sigma_H=-eB\left(\frac{e}{2\pi}\right)^2\oint dk_{\parallel}v_i\epsilon_{ik}m_{kl}^{-1}\epsilon_{lj}v_j\tau^2/v, \tag{4}$$

$$\beta=-e\mathcal{L}_0T\left(\frac{e}{2\pi}\right)^2\oint dk_{\parallel}v_im_{ij}^{-1}v_j\tau/v^3, \tag{5}$$

$$\Delta\sigma=-(eB)^2\left(\frac{e}{2\pi}\right)^2\oint dk_{\parallel}v_i\epsilon_{ik}m_{kn}^{-1}m_{nl}^{-1}\epsilon_{lj}v_j\tau^3/v, \tag{6}$$

expressed in terms of the inverse mass tensor $m_{ij}^{-1}=(\partial^2\varepsilon/\partial_{k_i}\partial_{k_j})$, the Levi-Civitá tensor ϵ_{ij}, and the Lorenz number $\mathcal{L}_0=\pi^2/3e^2$. The Fermi surface has been parametrized by arclength $k_\parallel$ and the two dimensional momentum integrals carried out as $\int d^2k\cdots=\int d\varepsilon\oint dk_\parallel/v\cdots$. The thermoelectric conductivity rests upon a first order expansion of the velocity in local momentum coordinates along the normal and tangential directions of the constant energy contours

$$v=v_F+\left(\frac{v_i}{v}\frac{\partial v_i}{\partial k_j}\frac{v_j}{v}\right)\delta k_\perp+\left(\frac{\epsilon_{ij}v_j}{v}\frac{\partial v_l}{\partial k_i}\frac{v_l}{v}\right)\delta k_\parallel, \tag{7}$$

where only the normal component proportional to $\delta\varepsilon=v\,\delta k_\perp$ provides a nonzero contribution to the thermoelectric conductivity.

In the case of an anisotropic relaxation time $\tau(\mathbf{k})$, the first three transport coefficients listed above are only modified by the fact that τ now depends on $k_\parallel$. Using a somewhat oversimplified momentum dependence of τ, the hot-spot Fermi surface is implemented via step functions for the flat parts and corners multiplied by $\tau_f=1/\eta T$ and $\tau_c=W_H/T^2$, respectively. These particular dependences are largely motivated by both the expected outcome in terms of the transport relaxation rates from Eq. (1) and the available (semi) microscopic calculations for Fermi surfaces with nearly flat parts, van Hove singularities, or in the presence of commensurate antiferromagnetic fluctuations. Introducing weight factors of the flat parts (see Fig. 1)

$$a=\frac{\oint_f dk_\parallel v}{\oint dk_\parallel v}, \tag{8}$$

$$b=\frac{\oint_f dk_\parallel(v_i\epsilon_{ik}m_{kl}^{-1}\epsilon_{lj}v_j)/v}{\oint dk_\parallel(v_i\epsilon_{ik}m_{kl}^{-1}\epsilon_{lj}v_j)/v}, \tag{9}$$

$$c=\frac{\oint_f dk_\parallel v_im_{ij}^{-1}v_j/v^3}{\oint dk_\parallel v_im_{ij}^{-1}v_j/v^3}, \tag{10}$$

the plasma frequency

$$\omega_p^2=\left(\frac{e}{2\pi}\right)^2\oint dk_\parallel v, \tag{11}$$

a generalized cyclotron frequency

$$\omega_H=\frac{-eB\oint dk_\parallel(v_i\epsilon_{ik}m_{kl}^{-1}\epsilon_{lj}v_j)/v}{\oint dk_\parallel v} \tag{12}$$

and the energy scale

$$\omega_0=\frac{\oint dk_\parallel v}{\oint dk_\parallel v_im_{ij}^{-1}v_j/v^3}, \tag{13}$$

which for an isotropic system reduces to the Fermi energy, the longitudinal, Hall and thermoelectric conductivities may be written as

$$\sigma=\omega_p^2[a\tau_f+(1-a)\tau_c], \tag{14}$$

$$\sigma_H=\omega_p^2\omega_H[b\tau_f^2+(1-b)\tau_c^2], \tag{15}$$

$$\beta=-(e\mathcal{L}_0T\omega_p^2/\omega_0)[c\tau_f+(1-c)\tau_c]. \tag{16}$$

It is the square symmetry which makes the $\partial_{k\parallel}\tau$ terms cancel in σ_H and with the expansion used in β no such terms appear in the first place. As for the magnetoconductivity, however, the integrand will in general acquire additional terms proportional to powers of $\partial_{k\parallel}\tau$, the contributions of which are beyond the underlying step function approximation for $\tau(\mathbf{k})$.

With temperature scales $T_a^*=[(1-a)/a]\eta W_H$, $T_b^*=[(1-b)/b]^{1/2}\eta W_H$ and $T_c^*=[(1-c)/c]\eta W_H$, Eqs. (14)–(16) lead to the following temperature dependences given by simple fractions:

$$\rho=\frac{\eta}{\omega_p^2 a}\frac{T}{1+T_a^*/T}, \tag{17}$$

$$\sigma_H=\frac{\omega_p^2\omega_H b}{\eta^2}\frac{1+(T_b^*/T)^2}{T^2}, \tag{18}$$

$$\cot\,\theta_H=\frac{\eta a}{\omega_H b}\frac{1+T_a^*/T}{1+(T_b^*/T)^2}T, \tag{19}$$

$$R_H=\frac{\omega_H b}{B\omega_p^2 a^2}\frac{1+(T_b^*/T)^2}{(1+T_a^*/T)^2}, \tag{20}$$

$$\beta=-\frac{e\mathcal{L}_0\omega_p^2 c}{\eta\omega_0}(1+T_c^*/T), \tag{21}$$

$$S=\frac{e\mathcal{L}_0 c}{\omega_0 a}\frac{1+T_c^*/T}{1+T_a^*/T}T. \tag{22}$$

Clearly the resistivity crosses over from T^2 to T when T rises above T_a^*, while $\cot\theta_H$ varies throughout T^n with $n=0,1,2,3$ but only as T^2 when $T\ll\min(T_a^*,T_b^*)$. The linear ρ and the quadratic $\cot\,\theta_H$ can only be attained asymptotically in the mutually excluding temperature ranges above and below T_a^*. Furthermore, R_H and σ_H will never exhibit the observed, simple power-law behaviors which are T^{-1} and T^{-3}, respectively. The thermopower is likely to come out linear in T and with the correct sign of the slope ($e<0$), however, the positive intercept observed in most experiments[15] is missing.

These general features may be illustrated in the concrete example of $YBa_2Cu_3O_7$, when using the band structure of Ref. 14 in a numerical parametrization of the Fermi surface. To fix the relative lengths of flat parts and corners, we rely on the fit to ac Hall data in Ref. 10 fixing b to 0.71. Since the ac data show more structure, this choice seems more reasonable than making an independent best fit of the resulting temperature dependences. With $b=0.71$, we find $a=0.88$ (consistent with Ref. 10) and $c=0.87$, implying that $T_a^*\approx T_c^*\approx 0.15\eta W_H$ and $T_b^*\approx 0.65\eta W_H$. Figure 2 shows the resulting temperature dependences of ρ, $\cot\,\theta_H$, and S, scaled to their values at room temperature an using $\eta=4.5$ and $W_H=82.5$ K consistent with the fit of the additive two-τ model to ac Hall data made in Ref. 10.

Although the plotted curves for the resistivity and the inverse Hall angle are close to the wanted dependences of Eq. (1) for the parameters given and the temperatures considered, the explicit expressions for $\rho(T)$ and $\cot\,\theta_H(T)$ from Eqs. (17) and (19) show that, strictly speaking, these resemblances can only occur in mutually excluding temperature ranges. Due to the proximity of a and c, the thermopower is largely linear in T but with zero intercept. With the neglect of the above-mentioned terms containing $\partial_{k\parallel}\tau$, the calculated magnetoresistivity $\Delta\rho/\rho=-\Delta\sigma/\sigma-\theta_H^2$ introduces an additional temperature scale T_d^* which we find to be $0.80\eta W_H$ in the example considered in Fig. 2. It varies as T^{-4} for $T\ll T_{a,b,c,d}^*$, again in approximate agreement with the experiment,[16] but it crosses over to T^{-2} as T rises above $T_{a,b,c,d}^*$.

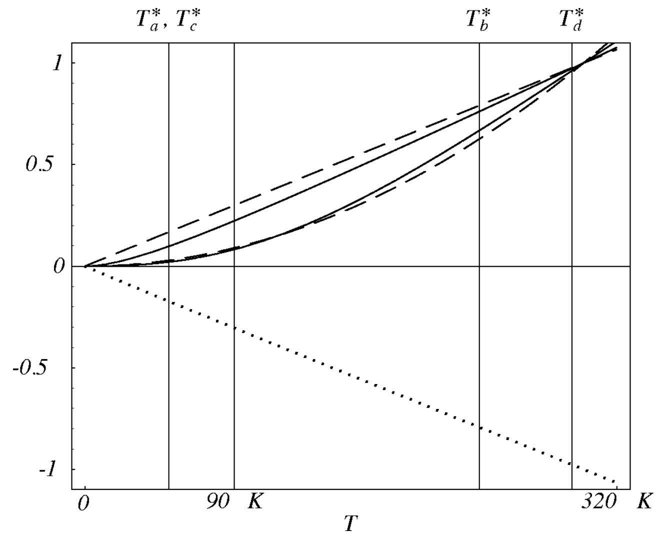

FIG. 2. $\rho(T)$ (upper full line), cot $\theta_H(T)$ (lower full line) and $S(T)$ (dotted line) normalized to their values at room temperature, calculated with an anisotropic scattering rate and using $\eta=4.5$ and $W_H=82.5$ K. Dashed lines show, respectively, $T/300$ K (upper) and $T^2/(300\text{ K})^2$ (lower) for comparison.

In Refs. 11 and 12 the additive two-τ approach was used together with Ong's formula for the Hall conductivity[17,16] as being equal to the area traced out by the mean free path vector as one circulates the Fermi surface. These areas were estimated to be proportional to $l_c l_f$ whereby $\sigma\propto l_f$ ensures that $\tan\,\theta_H\propto l_c$, in agreement with Eq. (1). We stress, however, that the exact area is given by the integral of l^2 which, in accordance with Eq. (15), yields a sum of squares of l_c and l_f rather than the product of the two.

A concrete realization of the hot-spot model is the nearly antiferromagnetic Fermi liquid (NAFL) (Ref. 18) (cf. also Ref. 19 for points much alike those being made here) in which the quasiparticle relaxation rate is determined by the coupling to antiferromagnetic spin fluctuations. In Ref. 18 the Hall conductivity was found to contain not only the T^{-4} and T^{-2} terms important, respectively, at low and high temperatures, but also a T^{-3} term which dominates in some intermediate range of temperatures. This crucial T^{-3} term appears to be a special feature of the NAFL model, but is not intrinsic to the two-τ approach which is based on the T-independent a and b.

It was pointed out by Hlubina and Rice[20] that for microscopic models featuring hot spots, the standard result for the resistivity consistent with Eq. (17) can be improved by using a *short-circuiting* variational solution of the Boltzmann equation much like $\mathbf{E}\cdot\mathbf{v}/(e^{|\Delta_{k_\parallel}|}+1)$, where $\Delta_{k_\parallel}$ is minimal on the cold corners, and vanishes all together when T increases above ηW_H where the two rates become equal. This distribution function favors the cold corners, enhances T_a^*, and extends the region of quadratic resistivity to even higher temperatures, thereby further reducing the potentiality of the hot spot model. It is worthwhile mentioning that the recent results of Boebinger *et al.*[21] indicate that the linear resistivity and quadratic cot θ_H observed at optimal doping indeed persist down to very low temperatures when suppressing superconductivity with a large pulsed magnetic field.

One might note that this short circuiting of the Fermi surface bears a certain resemblance to the behavior one would expect upon entering the underdoped region, where a d-wave pseudogap has been shown to evolve.[22] Thus, with a $d_{x^2-y^2}$-wave symmetric gap in the quasiparticle spectrum $E_k=\sqrt{\xi_k^2+\Delta_k^2}$, the conductivity will have enhanced weights on the nodal regions, which is again restricting the linear resistivity to higher temperatures. In the underdoped materials, a restriction of the linear resistivity to higher temperature is indeed observed, but rather as the top of an s-shaped curve, than as a tangent to the low temperature parabola found here.[23]

As for the vanishing intercept in the thermopower, one possible remedy of the above might be to use an energy dependent relaxation rate causing an additional term in β through the expansion of $\tau(\varepsilon)$. This remains to be resolved, though it has been suggested in Ref. 24 that spin fluctuations may accommodate just the right energy dependence of τ_c for the corners to yield the missing constant term.

To summarize, we have reinvestigated the hot-spot or additive two-τ model, with an emphasis on temperature dependences of galvanomagnetic and thermoelectric coefficients. In spite of a somewhat deceiving resemblance with the existing data, we find systematic deviations of these dependences from the simple power laws which have been found as approximately universal features of the normal state transport in optimally doped cuprates. As an immediate consequence of the explicit formulas of Eqs. (17)–(22), we note the unavoidable appearance of additional temperature scales ($T^*_{a,b,c,d}$), which to some extent obscures the original intention underlying the two-relaxation-time ansatz. The dependences given by Eqs. (17)–(22) should make it possible to contrast the experimental data against a generic additive two-τ model and to assess a general validity of such a phenomenological description.

The authors are grateful to V. M. Yakovenko, H. D. Drew, H. Smith, and A. Luther for valuable discussions.

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